WEST

End of Result Set

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L4: Entry 1 of 1

File: PGPB

Oct 3, 2002

DOCUMENT-IDENTIFIER: US 20020142108 A1

TITLE: Liquid crystal compounds, liquid crystal medium and liquid crystal display

Detail Description Table CWU (21):

25 Compound/Abbreviation Concentration/mass-% PTG-5-S 10.0 PTU-3-S 15.0 PTU-40-S 10.0 PVG-5-S 10.0 PGU-3-S 10.0 PPU-3-S 5.0 PPU-4-S 5.0 PPU-5-S 5.0 PGIP-3-N 15.0 PPYP-4N 15.0 .SIGMA. 100.0

Detail Description Table CWU (23):

27 Compound/Abbreviation Concentration/mass-% PTG-5-S 10.0 PTU-3-S 13.0 PTU-40-S 10.0 PVG-5-S 11.0 PGU-3-S 10.0 PPU-3-S 5.0 PPU-4-S 5.0 PPU-5-S 5.0 PGIP-3-N 12.0 PPYP-4N 13.0 PVG-V-S 6.0 .SIGMA. 100.0

```
313472-50-3 REGISTRY
RN
CN
```

Benzene, 1,3-difluoro-2-isothiocyanato-5-[(4-pentylphenyl)ethynyl]- (9CI)

(CA INDEX NAME)

3D CONCORD FS MF C20 H17 F2 N S

SR CA

STN Files: CA, CAPLUS, USPATFULL LC

Ring System Data

| | | | Ring System | | RID |
|----------|----------|------------|-------------|------------|------------|
| Analysis | Sequence | the Rings | Formula | Identifier | Occurrence |
| EA | ES | SZ | RF | RID | Count |
| ======== | +======= | +========- | }========= | }======== | -======== |
| C6 | C6 | 6 | C6 | 46.150.18 | 2 |

Calculated Properties (CALC)

| PROPERTY (CODE) | VALUE | CONDITION | NOTE |
|---|--------------------|------------------|---------|
| ======================================= | +============ | +======= | |
| Bioconc. Factor (BCF) | 1396095 | pH 1 | (1) ACD |
| Bioconc. Factor (BCF) | 1396095 | pH 4 | (1) ACD |
| Bioconc. Factor (BCF) | 1396095 | pH 7 | (1) ACD |
| Bioconc. Factor (BCF) | 1396095 | pH 8 | (1) ACD |
| Bioconc. Factor (BCF) | 1396095 | pH 10 | (1) ACD |
| Boiling Point (BP) | 450.7+/-35.0 deg C | | |
| Enthalpy of Vap. (HVAP) | 68.24+/-3.0 kJ/mol | | (1) ACD |
| Flash Point (FP) | 226.4+/-46.7 deg C | | (1) ACD |
| H acceptors (HAC) | 1 | | (1) ACD |
| H donors (HD) | İo | | (1) ACD |
| Koc (KOC) | 871159 | pH 1 | (1) ACD |
| Koc (KOC) | 871159 | рН 4 | (1) ACD |
| Koc (KOC) | 871159 | рн 7 | (1) ACD |
| Koc (KOC) | 871159 | 8 Hq | (1) ACD |
| Koc (KOC) | 871159 | pH 10 | (1) ACD |
| logD (LOGD) | 8.39 | pH 1 | (1) ACD |
| logD (LOGD) | 8.39 | pH 4 | (1) ACD |
| logD (LOGD) | 8.39 | pH 7 | (1) ACD |
| logD (LOGD) | 8.39 | рн 8 | (1) ACD |
| logD (LOGD) | 8.39 | рH 10 | (1) ACD |
| logP (LOGP) | 8.388+/-0.512 | - | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 1 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 4 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | рн 7 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | рн 8 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD |
| Molecular Weight (MW) | 341.42 | i ⁻ i | (1) ACD |
| Vapor Pressure (VP) | 6.87E-08 Torr | 25.0 deg C | (1) ACD |
| | • | ' | • |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris

4 REFERENCES IN FILE CA (1957 TO DATE) 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 4 REFERENCES IN FILE CAPLUS (1957 TO DATE) REFERENCE 1 ΑN 136:110201 CA ΤI Liquid crystal compound, nematic liquid crystal mixture, and polymer dispersion liquid crystal display Poetsch, Eike; Meyer, Volker; Krause, Joachim; Manabe, Atsutaka IN Merck Patent G.M.B.H., Germany PA Jpn. Kokai Tokkyo Koho, 40 pp. SO CODEN: JKXXAF DT Patent LA Japanese IC ICM C09K019-42 ICS C09K019-12; C09K019-16; C09K019-30; G02F001-13; G02F001-1334 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes) Section cross-reference(s): 75 FAN.CNT 1 KIND DATE APPLICATION NO. DATE PATENT NO. ----------______ JP 2002012871 A2 20020115 JP 2001-137750 20010508 PΙ PRAI EP 2000-109163 20000508 The invention relates to a nematic liq. crystal mixt. contg. a pos. anisotropic compd.(s) showing .DELTA.n of .gtoreq.0.30 (at 20.degree., 589.3 nm) represented by R1-A11-Z11-[A12-Z12]n-A13-NCS (R1 = C1-12-alky, Cl, OCF3, CN, NCS, F; Z11, Z12 = trans-CH:CH-, -CH:CF-, -CF:CH-, -CF:CF-, single bond; Al1 = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-phenylene with F-substituent(s); A12, A13 = 1,4-phenylene, 1,4-phenylene with F-substituent(s); n = 0, 1) and a pos. anisotropic compd.(s) represented by R2-[A21]n-A22-A23-X2 (R2 = C1-12-alky, C1, OCF3, CN, NCS, F; Z11, Z12 = C1-12-alky) trans-CH:CH-, -CH:CF-, -CF:CH-, -CF:CF-, single bond; A21 = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-phenylene with F-substituent(s); A22, A23 = 1,4-phenylene, 1,4-phenylene with F-substituent(s); X2 = CN, F, Cl; n = 0, 1). The liq. crystal mixt., showing wide-nematic-phase temp. ranges and low viscosity, is esp. suitable for (holog.) polymer dispersed liq. crystal displays. ST nematic liq crystal mixt polymer dispersion display IT Liquid crystal displays (nematic liq. crystal mixt. esp. suitable for holog. polymer dispersion liq. crystal display) IT Liquid crystals (nematic; nematic liq. crystal mixt. esp. suitable for holog. polymer dispersion liq. crystal display) TΤ 38190-45-3 40817-08-1 52709-86-1 54211-46-0 63617-61-8 99217-32-0 104569-88-2 116831-09-5 104569-87-1 99602-91-2 132123-39-8 137019-94-4 137019-95-5 219939-28-3 219939-29-4 356797-92-7 281680-31-7 313472-50-3 316364-68-8 356797-91-6 356797-97-2 356797-99-4 356798-03-3 356797-93-8 356798-05-5 356798-06-6 356798-12-4 356798-23-7 356798-25-9 356798-26-0 356798-31-7 385435-70-1 356798-27-1 356798-32-8 388625-24-9 388625-26-1 388625-28-3 388625-29-4 388625-25-0 388625-31-8 388625-33-0 388625-42-1 388625-45-4 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses) (nematic liq. crystal mixt. esp. suitable for holog. polymer dispersion liq. crystal display) 288-32-4, Imidazole, reactions 463-71-8, Thiophosgene TΤ 6160-65-2 67567-26-4, 4-Bromo-2,6-difluoroaniline 143651-26-7, Boronic acid,

[4-(4-pentylcyclohexyl)phenyl]-, trans- 388623-07-2

388623-85-6

```
RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of nematic liq. crystal mixt. esp. suitable for holog. polymer
        dispersion liq. crystal display)
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ΙT
     138074-14-3P
                    385435-64-3P
                                   385435-68-7P
                                                  385435-69-8P
                    388623-10-7P
                                   388623-12-9P
                                                 388623-13-0P
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                                                 388624-99-5P
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                                  388625-03-4P
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                                  388625-08-9P
                                                 388625-09-0P
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                   388625-17-0P
     388625-16-9P
                                  388625-18-1P
                                                 388625-19-2P
                                                                388625-20-5P
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                                  388625-23-8P
     RL: SPN (Synthetic preparation); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
        (prepn. of nematic liq. crystal mixt. esp. suitable for holog. polymer
        dispersion liq. crystal display)
REFERENCE 2
AN
     136:77327 CA
    Liquid-crystal medium, liquid-crystal display using it, and utilization of
TI
    Manabe, Atsutaka; Poetsch, Eike; Reiffenrath, Volker
IN
    Merck Patent G.M.B.H., Germany
PA
SO
     Jpn. Kokai Tokkyo Koho, 27 pp.
     CODEN: JKXXAF
DT
    Patent
LA
    Japanese
IC
     ICM C09K019-02
         C09K019-12; C09K019-16; C09K019-18; C09K019-30; C09K019-34;
         C09K019-42; G02F001-13; G02F001-1334
CC
    74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other
    Reprographic Processes)
FAN.CNT 1
```

APPLICATION NO. DATE

PATENT NO.

KIND DATE

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JP 2002003844
                      A2
                            20020109
                                           JP 2001-137708
                                                            20010508
PΤ
PRAI EP 2000-109162
                      20000508
     The medium contains (1) a strongly pos. dielec. liq.-crystal component A
     comprising .gtoreq.1 compds. having NCS groups at a terminal and having
     .DELTA.n >0.30 at 20.degree. and 589.3 nm and (2) a pos. dielec.
     liq.-crystal component B contg. compds. with broad nematic phase range.
     Also claimed are liq.-crystal displays and systems including the medium.
     The medium is esp. suitable for polymer dispersed liq.-crystal systems
     (PDLC) and holog. PDLC.
ST
     liq crystal display pos dielec component broad nematic phase
IT
     Liquid crystal displays
        (liq.-crystal medium with strongly pos. dielec. and broad nematic phase
        range for display)
IT
     40817-08-1D, mixt. contq.
                                 52709-86-1D, mixt. contq.
                                                             58743-75-2D, mixt.
     contg. 58743-76-3D, mixt. contg. 99217-32-0D, mixt. contg.
     116831-09-5D, mixt. contg. 138074-14-3D, mixt. contg.
                                                               313472-50-3D,
                  316364-68-8D, mixt. contg.
     mixt. contg.
                                                356797-91-6D, mixt. contg.
     356797-92-7D, mixt. contg. 356797-93-8D, mixt. contg.
                                                               356797-99-4D,
     mixt. contg. 356798-03-3D, mixt. contg. 356798-05-5D, mixt. contg.
                                356798-23-7D, mixt. contg.
     356798-06-6D, mixt. contg.
                                                               356798-27-1D,
     mixt. contg. 385435-48-3 385435-64-3D, mixt. contg. 385435-68-7D mixt. contg. 385435-69-8D, mixt. contg. 385435-70-1D, mixt. contg.
                                  385435-64-3D, mixt. contg.
                                                               385435-68-7D,
     385435-71-2 385435-72-3 385435-73-4D, mixt. contg.
     RL: DEV (Device component use); TEM (Technical or engineered material
     use); USES (Uses)
        (liq.-crystal medium with strongly pos. dielec. and broad nematic phase
        range for display)
REFERENCE 3
AN
     135:203078 CA
TI
     Liquid crystal medium comprising strongly dielectric positive
     isothiocyanate compound for polymer dispersed liquid crystal display
     Poetsch, Eike; Manabe, Atsutaka; Reiffenrath, Volker; Reuter, Markus;
IN
     Krause, Joachim; Pauluth, Detlef
PΑ
     Merck Patent Gmbh, Germany
SO
     Eur. Pat. Appl., 54 pp.
     CODEN: EPXXDW
DT
     Patent
     English
LA
IC
     ICM C09K019-02
         C09K019-16; C09K019-12; C09K019-42; C09K019-44; C09K019-54;
          C07C331-28
CC
     74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other
     Reprographic Processes)
     Section cross-reference(s): 75
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                           APPLICATION NO. DATE
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                                           -----
PΤ
    EP 1126006
                                           EP 2001-101157
                      A2
                            20010822
                                                            20010123
     EP 1126006
                     A3
                            20030226
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
          · IE, SI, LT, LV, FI, RO
                     A1 20021003
     US 2002142108
                                           US 2001-773673
                                                            20010202
                                           JP 2001-37730
     JP 2001254080
                      A2---20010918
                                                            20010214
PRAI EP 2000-102952 20000214
    EP 2000-109164
                     20000508
     EP 2000-126408
                     20001205
     EP 2000-EP00109164 20000508
     EP 2000-EP00126408 20001205
```

$$R^1$$
 A^1 Z^1 A^2 Z^2 A^3 NCS NCS NCS NCS

- The invention relates to liq. crystal media comprising a strongly dielec. pos. isothiocyanate compds. of formula I (R1=alkyl, C1-10-alkoxy, alkenyl, C1-7-alkenyloxy or-alkoxyalkyl, CN, NCS, halogen; Z1, Z2 = single bond, trans-CH=CH, Z2 = single bond if n1 = 0; n1 = 0,1; A1, A2, A3 = phenyls, at least one of phenyls is substituted by one or two fluorine atoms), and another dielec. pos. compd., preferably comprising terminally polar substituted bi- or terphenyl compds., as further defined in the claims, as well as to liq. crystal displays comprising these media, in particular to polymer dispersed liq. crystal display (PDLC) and most particular to holog. PDLC displays.
- ST liq crystal isothiocyanate compd medium prepn polymer dispersed display

IT Liquid crystal displays

Liquid crystals

(liq. crystal medium comprising strongly dielec. pos. isothiocyanate compds for polymer dispersed liq. crystal display)

IT 92-52-4, Biphenyl, reactions 367-24-8, 4-Bromo-2-fluoroaniline 461-961, 1-Bromo-3,5-difluoro-benzene 588-96-5, p-Ethoxyphenylbromide
5459-40-5, 4-Ethoxy-styrene 6160-65-2 6163-58-2, Tri-o-tolylphosphine
10101-89-0, Trisodiumphosphate dodecahydrate 13965-03-2 23055-77-8,
4-Bromo-4'-chloro-biphenyl 31989-57-8, Bis(triphenylphosphine) palladium
67567-26-4, 4-Bromo-2,6-difluoroaniline 105931-73-5,

1-Bromo-3-fluoro-4-iodo-benzene

RL: RCT (Reactant); RACT (Reactant or reagent)

(in prepn. of isothiocyanate liq. crystal compds)

IT 71274-84-5P, 4-Trifluoromethoxy-biphenyl

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in prepn. of isothiocyanate liq. crystal compds)

356797-92-7P 356797-93-8P 356797-94-9P IT 160347-36-4P 356797-91-6P 356797-96-1P 356797-97-2P 356797-98-3P 356797-99-4P 356797-95-0P 356798-01-1P 356798-02-2P 356798-03-3P 356798-04-4P 356798-00-0P 356798-07-7P 356798-09-9P 356798-05-5P 356798-06-6P 356798-08-8P 356798-13-5P 356798-11-3P 356798-12-4P 356798-14-6P 356798-10-2P 356798-17-9P 356798-18-0P 356798-15-7P 356798-16-8P 356798-19-1P 356798-21-5P 356798-22-6P 356798-20-4P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(liq. crystal medium comprising strongly dielec. pos. isothiocyanate compds for polymer dispersed liq. crystal display)

219939-29-4 ΤТ 63617-61-8 116831-09-5 127523-43-7 219939-28-3 356798-26-0 313472-50-3 356798-23-7 356798-24-8 356798-25-9 356798-28-2 356798-29-3 356798-30-6 356798-31-7 356798-27-1 356798-32-8

RL: TEM (Technical or engineered material use); USES (Uses) (liq. crystal medium comprising strongly dielec. pos. isothiocyanate compds for polymer dispersed liq. crystal display)

REFERENCE 4

- AN 134:63754 CA
- TI Materials for liquid crystal displays with reduced power consumption
- AU Kirsch, Peer; Bremer, Matthias; Kirsch, Annette; Manabe, Atsutaka; Poetsch, Eike; Reiffenrath, Volker; Tarumi, Kazuaki
- CS Liquid Crystals Division, Merck KGaA, Darmstadt, 64271, Germany
- SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2000), 346, 193-199
 CODEN: MCLCE9; ISSN: 1058-725X

- PB Gordon & Breach Science Publishers
- DT Journal
- LA English
- CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75
- AB A significant redn. of the power consumption of a liq. crystal display can be achieved either by application of a lower driving voltage or even more effectively by use of a holog. structured reflective scattering type of display without color filters. The first option requires strongly polar materials with extremely high reliability, the second one new types of liq. crystals with a birefringence as high as possible in order to optimize the scattering effect. A mol. modeling based method for the prediction of reliability parameters is presented.
- ST liq crystal display active matrix high birefringence reliability material; mol model stable materials liq crystal display active matrix
- IT Liquid crystal displays

(active matrix; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption)

IT Ion-molecule reaction

(enthalpy, calcd. semiempirical; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)

IT Liquid crystals

(fluorinated; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)

IT Reaction enthalpy

(ion-mol. reaction, calcd. semiempirical; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)

IT Impurities

(ionic; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)

IT Birefringence

Dielectric anisotropy

(materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption)

IT Molecular modeling

(materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption supported by)

IT Molecular structure-property relationship

(stability; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to materials stability)

IT 126391-77-3 133261-31-1 221526-80-3 255728-73-5 255728-82-6 308117-08-0 313472-49-0 313472-50-3

RL: PRP (Properties)

(materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption)

IT 17341-25-2, processes

RL: PEP (Physical, engineering or chemical process); PROC (Process) (materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to ionic impurities)

- RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
- (1) Bremer, M; Adv Mater 1993, V5, P842 CAPLUS
- (2) Bremer, M; Jpn J Appl Phys 1998, V37, PL88 CAPLUS
- (3) Kirsch, P; Angew Chem 1999, V111, P2174
- (4) Kirsch, P; Angew Chem Int Ed Engl 1999, V38, P1989 CAPLUS
- (5) Klasen, M; Jpn J Appl Phys 1998, V37, PL945 CAPLUS

(6) Sasaki, A; Japan Display '86 1986, P62

```
1993:59406 CAPLUS
AN
     118:59406
DN
     2,6 difluorotolane
TI
     Reiffenrath, Volker; Plach, Herbert
ΙN
     Merck Patent G.m.b.H., Germany
PA
     Ger. Offen., 19 pp.
so
     CODEN: GWXXBX
DT
     Patent
LA
     German
TC
     ICM C07C043-225
         C07C025-24; C09K019-06; G09F009-35; G02F001-13; C07D319-06;
     TCS
          C07D213-24; C07D239-24
     C09K019-18; C09K019-30; C09K019-34; C09K019-20; C09K019-58; C07D521-00;
     C07D401-10; C07D401-12; C07D405-10; C07D405-12
     25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                           APPLICATION NO. DATE
                     _ _ _ _
                            _____
                                           -----
                                           DE 1991-4105742 19910223
PΙ
     DE 4105742
                      A1
                            19920827
     DE 4105742
                      C2
                            20010809
PRAI DE 1991-4105742
                            19910223
     CASREACT 118:59406; MARPAT 118:59406
GT
```

$$R^{1}(A^{1}-Z^{1})n$$

$$F$$
 $C \equiv C$

$$(Z^{2}-A^{2})mR^{2}$$

AB A process was developed for the prepn. of 2,6-difluorotolane of formula I [R1, R2 = alkyl or alkenyl, A1, A2 = 1,4-cyclohexylene, -phenylene, 2- or 3-fluoro-1,4-phenylene, Z1, Z2 = CH2CH2, -CH2O-, (CH2)4, m, n, o = 1-2] as a component of liq. crystal medium having electrooptical properties. E.g., the treatment of 3,5-difluoropentylbenzene (0.129 mol) with 114 mL THF and BuLi followed by 4-ethoxyacetophenone (0.129 mol) gave a product mixt. which was treated with p-toluenesulfonic acid (4 g) in toluene. Subsequent reaction of product mixt. with .09 mL bromine in EtOAc and with 12.6 mL Et3N and then reaction with LDA in THF gave final product 4-pentyl-2,6-difluoro-4'-ethoxytolane.

ST fluorotolane electrooptical property; acetylene difluoro diphenyl; palladium catalyst coupling fluorophenylacetylene iodobenzene

IT Coupling reaction

(of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT Coupling reaction catalysts

(palladium compds., for the coupling of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT 144890-97-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(3)

IT 14221-01-3

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for the coupling of difluoroiodobenzene derivs. with fluorophenylacetylene)

IT 13965-03-2

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for the coupling of difluorophenylacetylene deriv. with trifluoromethoxyiodobenzene)

```
IT
     628-17-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with difluorobromobenzene)
IT
     461-96-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with iodopentane)
IT
     103962-05-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (coupling reaction of, with difluorophenylacetylene deriv.)
IT
     766-98-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (coupling reaction of, with ethoxydifluoroiodobenzene)
TT
     144911-50-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (coupling reaction of, with trifluoromethoxyiodobenzene)
IT
     144891-25-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (iodination of)
IT
     144891-24-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and coupling of, with fluorophenylacetylene)
                                  52709-83-8P
                                                58743-75-2P
                                                               58743-76-3P
IT
     40817-08-1P
                   41122-70-7P
                                                               80955-71-1P
                                                80944-44-1P
     61203-99-4P
                   61204-01-1P
                                  79832-84-1P
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                                                 144890-96-0P
                                  134143-76-3P
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                   85600-56-2P
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                                    144891-01-0P
                                                                   144891-03-2P
     144890-99-3P
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     144891-09-8P
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                    144891-43-0P
                                    144891-44-1P
                                                   144891-45-2P
                                                                   144891-46-3P
                    144891-48-5P
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     144891-47-4P
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                    144891-63-4P
                                    144891-64-5P
                                                   144891-65-6P
                                                                   144891-66-7P
     144891-67-8P
                    144891-68-9P
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     144891-77-0P
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                    144892-08-0P
                                    144892-09-1P
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                    144892-28-4P
                                    144892-29-5P
                                                   144892-30-8P
                                                                   144892-31-9P
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                    144892-33-1P
                                    144892-34-2P
                                                   144892-35-3P
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     144892-37-5P
                    144892-38-6P
                                    144892-39-7P
                                                   144892-40-0P
                                                                   144892-41-1P
                    144892-43-3P
                                    144892-44-4P
                                                   144892-45-5P
                                                                   144892-46-6P
     144892-42-2P
     144892-47-7P
                    144892-48-8P
                                    144892-49-9P
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                    144892-53-5P
                                    144892-54-6P
                                                   144892-55-7P
                                                                   144892-56-8P
     144892-52-4P
     144892-57-9P
                    144892-58-0P
                                    144892-59-1P
                                                   144892-60-4P
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                    144892-63-7P
                                    144911-05-7P
                                                   144911-06-8P
                                                                   144911-07-9P
     144892-62-6P
     144911-08-0P
                    144911-09-1P
                                    144911-10-4P
                                                   144911-11-5P
                                                                   144911-12-6P
     144911-13-7P
                    144911-14-8P
                                    144911-15-9P
                                                   144911-16-0P
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     144911-18-2P
                    144911-19-3P
                                    144911-20-6P
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                                                                   144911-22-8P
     144911-23-9P
                    144911-24-0P
                                    144911-25-1P
                                                   144911-26-2P
                                                                   144911-27-3P
     144911-28-4P
                    144911-29-5P
                                    144911-30-8P
                                                   144911-31-9P
                                                                   144911-32-0P
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144911-35-3P
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     144911-33-1P
                    144911-34-2P
                                                                  144911-37-5P
     144911-38-6P
                    144911-39-7P
                                    144911-40-0P
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                                                                  144911-42-2P
     144911-43-3P
                    144911-44-4P
                                    144911-45-5P
                                                   144911-46-6P
                                                                  144911-47-7P
     144911-48-8P
                    144911-49-9P
                                    144911-51-3P
                                                   144911-52-4P
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     144911-54-6P
                    144911-55-7P
                                    144911-56-8P 144911-57-9P
     144911-58-0P 144911-59-1P 144911-60-4P
     144911-61-5P 144911-62-6P 144911-63-7P
                    144911-65-9P
     144911-64-8P
                                   144911-66-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
TΤ
     144911-67-1P
                    144911-68-2P
                                    144911-69-3P
                                                   144911-70-6P
                                                                  144911-71-7P
     144911-72-8P
                    144911-73-9P
                                   144911-74-0P
                                                   144922-37-2P
                                                                  144922-38-3P
     144922-39-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
IT
     1676-63-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with difluoro(pentyl)benzene)
IT
     121219-25-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with ethoxyacetophenone)
IT
     144891-33-8P 144891-34-9P 144891-35-0P
     144891-36-1P 144891-37-2P 144891-38-3P
     144891-39-4P 144911-57-9P 144911-58-0P
     144911-59-1P 144911-60-4P 144911-61-5P
     144911-62-6P 144911-63-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     144891-33-8 CAPLUS
     Benzene, 5-ethoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-
CN
     (9CI) (CA INDEX NAME)
```

$$c \equiv c$$
 $c = c$
 $c = c$
 $c = c$

RN 144891-34-9 CAPLUS
CN Benzene, 1,3-difluoro-5-propoxy-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 $$c = c$$
 $c = c$
 $c =$

RN 144891-36-1 CAPLUS

CN Benzene, 5-ethyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 $c = c$
 $c = c$

RN 144891-37-2 CAPLUS

CN Benzene, 1,3-difluoro-5-propyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 $c = c$
 $c = c$
 $c = c$

RN 144891-38-3 CAPLUS

CN Benzene, 5-butyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 $c = c$
 $c = c$
 $c = c$

RN 144891-39-4 CAPLUS

CN Benzene, 1,3-difluoro-5-pentyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$C = C$$

Me- (CH₂) 4

F

O- CF₃

RN 144911-57-9 CAPLUS

CN Benzene, 1,3-difluoro-5-hexyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-(9CI) (CA INDEX NAME)

RN 144911-58-0 CAPLUS

CN Benzene, 1,3-difluoro-5-heptyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

RN 144911-59-1 CAPLUS

CN Benzene, 1,3-difluoro-5-octyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$C = C$$

Me- (CH_2) 7

F

O- CF_3

RN 144911-60-4 CAPLUS

CN Benzene, 1,3-difluoro-5-(pentyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$C = C$$

Me- $(CH_2)_4$ -0

F

O-CF₃

RN 144911-61-5 CAPLUS

CN Benzene, 1,3-difluoro-5-(hexyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

RN 144911-62-6 CAPLUS

CN Benzene, 1,3-difluoro-5-(heptyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

RN 144911-63-7 CAPLUS

CN Benzene, 1,3-difluoro-5-(octyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-(9CI) (CA INDEX NAME)

$$C = C$$

Me- (CH₂)₇-0

F

O-CF₃

```
AN 1990:641336 CAPLUS
```

- DN 113:241336
- TI Synthesis and properties of liquid crystalline materials with high optical anisotropy
- AU Reiffenrath, V.; Finkenzeller, U.; Poetsch, E.; Rieger, B.; Coates, D.
- CS Ind. Chem. Div., E. Merck, Darmstadt, D-6100, Germany
- SO Proceedings of SPIE-The International Society for Optical Engineering (1990), 1257(Liq. Cryst. Disp. Appl.), 84-94
 CODEN: PSISDG; ISSN: 0277-786X
- DT Journal
- LA English
- CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 21, 75
- AB The introduction of F and F-contg. substituents in the terminal position of high .DELTA.n (refractive index difference) materials leads to liq. crystals with high pos. dielec. anisotropy and low viscosity. These liq. crystals exhibit high resistivity and excellent UV-stability. In contrast to the cyano-substituent these moieties do not enhance the optical anisotropy; therefore the use of basic structures having high optical anisotropy such as tolanes and terphenyls is necessary. In the case of terphenyls the introduction of an ethylenic bridge in addn. to lateral fluorination leads to mols. having a wide nematic phase range.
- ST synthesis liq crystal optical anisotropy; electrooptical device liq crystal dielec anisotropy
- IT Liquid crystals

(prepn. of fluorine-contg., with high optical anisotropy and UV stability and low viscosity)

IT Optical imaging devices

(electro-, liq.-crystal, prepn. of fluorine-contg. liq. crystal materials having high optical anisotropy and UV stability and low viscosity for)

IT 95759-62-9P 116903-47-0P 121218-93-7P 130746-59-7P

130746-60-0P 130746-61-1P 130746-62-2P

130746-63-3P 130746-64-4P 130746-65-5P 130746-66-6P

130746-67-7P 130746-68-8P 130746-69-9P 130746-70-2P 130746-71-3P 130746-72-4P 130746-73-5P 130746-74-6P 130746-75-7P 130746-76-8P

130746-77-9P 130746-78-0P 130746-79-1P 130746-80-4P 130746-81-5P

RL: PREP (Preparation)

(prepn. and dielec. anisotropy and UV stability and viscosity of, for display devices)

IT 130746-60-0P 130746-62-2P 130746-63-3P

RL: PREP (Preparation)

(prepn. and dielec. anisotropy and UV stability and viscosity of, for display devices)

- RN 130746-60-0 CAPLUS
- CN Benzene, 1-[(4-pentylphenyl)ethynyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

hot

RN 130746-62-2 CAPLUS

CN Benzene, 1-[(4-butoxyphenyl)ethynyl]-4-(trifluoromethoxy)- (9CI) INDEX NAME)

) (C#

at my

RN 130746-63-3 CAPLUS

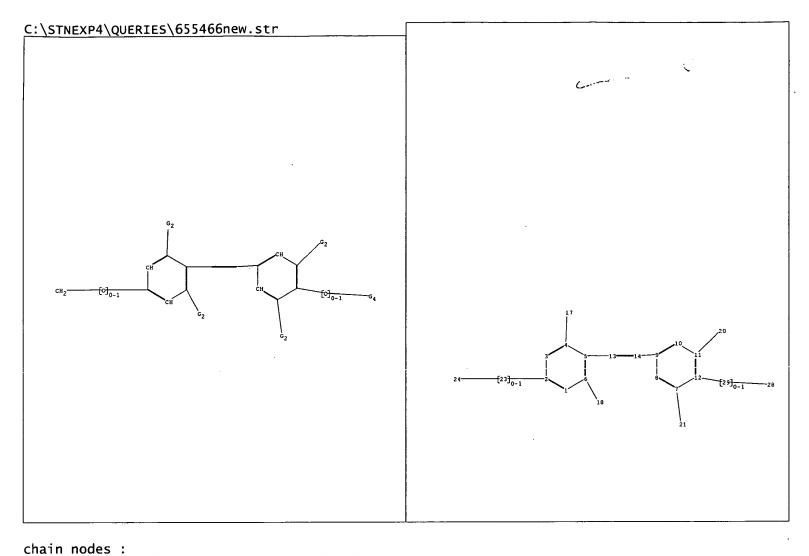
CN Benzene, 1-[(4-butoxyphenyl)ethynyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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C:\STNEXP4\QUERIES\655466a.str
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```
chain nodes :
   13 14 16 18 19 21 22 24 27 28
ring nodes : ___1_2_3 4 5 6 7 8
                        9 10 11 12
chain bonds :
   2-27 4-18 5-13 6-19 7-22 9-14 11-21 12-24 13-14 16-24 27-28
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
   2-27 4-18 6-19 7-22 11-21 12-24 16-24
exact bonds :
   5-13 9-14 13-14 27-28
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
G1:C,0
G2:H,F
```

G3:CF3.N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS 27:CLASS 28:CLASS



```
13 14 17 18 20 21 23 24 28 29

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds:

2-23 4-17 5-13 6-18 7-21 9-14 11-20 12-29 13-14 23-24 28-29

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds:

2-23 4-17 6-18 7-21 11-20 12-29 28-29

exact bonds:

5-13 9-14 13-14 23-24

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:C,0
```

G2:H,F

G3:CN,CF3,N

G4:CF3,N

Match level:
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 23:CLASS 24:CLASS 28:CLASS 29:CLASS

```
1993:59406 CAPLUS
AN
     118:59406
DN
TI
     2,6 difluorotolane
     Reiffenrath, Volker; Plach, Herbert
ΤN
PA
     Merck Patent G.m.b.H., Germany
SO
     Ger. Offen., 19 pp.
     CODEN: GWXXBX
DT
     Patent
     German
LA
IC
     ICM C07C043-225
         C07C025-24; C09K019-06; G09F009-35; G02F001-13; C07D319-06;
          C07D213-24; C07D239-24
     C09K019-18; C09K019-30; C09K019-34; C09K019-20; C09K019-58; C07D521-00;
ICA
     C07D401-10; C07D401-12; C07D405-10; C07D405-12
CC
     25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO. DATE
                     ----
                                           DE 1991-4105742 19910223
PΤ
     DE 4105742
                      Δ1
                            19920827
     DE 4105742
                       C2
                            20010809
PRAI DE 1991-4105742
                            19910223
     CASREACT 118:59406; MARPAT 118:59406
OS
GI
```

$$R^{1}(A^{1}-Z^{1})_{n} \longrightarrow C \equiv C \longrightarrow (Z^{2}-A^{2})_{m}R^{2}$$

AB A process was developed for the prepn. of 2,6-difluorotolane of formula I [R1, R2 = alkyl or alkenyl, A1, A2 = 1,4-cyclohexylene, -phenylene, 2- or 3-fluoro-1,4-phenylene, Z1, Z2 = CH2CH2, -CH2O-, (CH2)4, m, n, o = 1-2] as a component of liq. crystal medium having electrooptical properties. E.g., the treatment of 3,5-difluoropentylbenzene (0.129 mol) with 114 mL THF and BuLi followed by 4-ethoxyacetophenone (0.129 mol) gave a product mixt. which was treated with p-toluenesulfonic acid (4 g) in toluene. Subsequent reaction of product mixt. with .09 mL bromine in EtOAc and with 12.6 mL Et3N and then reaction with LDA in THF gave final product 4-pentyl-2,6-difluoro-4'-ethoxytolane.

ST fluorotolane electrooptical property; acetylene difluoro diphenyl; palladium catalyst coupling fluorophenylacetylene iodobenzene

IT Coupling reaction

(of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from) $\begin{tabular}{ll} \end{tabular}$

IT Coupling reaction catalysts

(palladium compds., for the coupling of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT 144890-97-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(3)

IT 14221-01-3

RL: CAT (Catalyst use); USES (Uses) (catalyst, for the coupling of difluoroiodobenzene derivs. with fluorophenylacetylene)

IT 13965-03-2

RL: CAT (Catalyst use); USES (Uses) (catalyst, for the coupling of difluorophenylacetylene deriv. with trifluoromethoxyiodobenzene)

```
IT
     628-17-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with difluorobromobenzene)
IT
     461-96-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with iodopentane)
TT
     103962-05-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (coupling reaction of, with difluorophenylacetylene deriv.)
IT
     766-98-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (coupling reaction of, with ethoxydifluoroiodobenzene)
TT
     144911-50-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (coupling reaction of, with trifluoromethoxyiodobenzene)
IT
     144891-25-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (iodination of)
IT
     144891-24-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and coupling of, with fluorophenylacetylene)
                   41122-70-7P
                                  52709-83-8P
IT
     40817-08-1P
                                                58743-75-2P
                                                               58743-76-3P
                                                               80955-71-1P
     61203-99-4P
                   61204-01-1P
                                  79832-84-1P
                                                80944-44-1P
                                  134143-76-3P
                                                 144890-96-0P
     81936-32-5P
                   85600-56-2P
                                                                 144890-98-2P
                                                   144891-02-1P
     144890-99-3P
                    144891-00-9P
                                    144891-01-0P
                                                                   144891-03-2P
                                    144891-06-5P
                                                   144891-07-6P
     144891-04-3P
                    144891-05-4P
                                                                   144891-08-7P
     144891-09-8P
                    144891-10-1P
                                    144891-11-2P
                                                   144891-12-3P
                                                                   144891-13-4P
     144891-14-5P
                    144891-15-6P
                                    144891-16-7P
                                                   144891-17-8P
                                                                   144891-18-9P
     144891-19-0P
                    144891-20-3P
                                                   144891-22-5P
                                    144891-21-4P
                                                                   144891-23-6P
                                    144891-28-1P
     144891-26-9P
                    144891-27-0P
                                                   144891-29-2P
                                                                   144891-30-5P
     144891-31-6P
                    144891-32-7P 144891-33-8P 144891-34-9P
     144891-35-0P 144891-36-1P 144891-37-2P
                                  144891-40-7P
     144891-38-3P 144891-39-4P
                                                 144891-41-8P
                    144891-43-0P
                                    144891-44-1P
     144891-42-9P
                                                   144891,-45-2P
                                                                   144891-46-3P
                    144891-48-5P
     144891-47-4P
                                    144891-49-6P
                                                   144891-50-9P
                                                                   144891-51-0P
     144891-52-1P
                    144891-53-2P
                                    144891-54-3P
                                                   144891-55-4P
                                                                   144891-56-5P
     144891-57-6P
                    144891-58-7P
                                    144891-59-8P
                                                   144891-60-1P
                                                                   144891-61-2P
     144891-62-3P
                    144891-63-4P
                                    144891-64-5P
                                                   144891-65-6P
                                                                   144891-66-7P
     144891-67-8P
                    144891-68-9P
                                    144891-69-0P
                                                   144891-70-3P
                                                                   144891-71-4P
     144891-72-5P
                    144891-73-6P
                                    144891-74-7P
                                                   144891-75-8P
                                                                   144891-76-9P
     144891-77-0P
                    144891-78-1P
                                    144891-79-2P
                                                   144891-80-5P
                                                                   144891-81-6P
     144891-82-7P
                    144891-83-8P
                                    144891-84-9P
                                                   144891-85-0P
                                                                   144891-86-1P
     144891-87-2P
                    144891-88-3P
                                    144891-89-4P
                                                   144891-90-7P
                                                                   144891-91-8P
     144891-92-9P
                    144891-93-0P
                                                   144891-95-2P
                                    144891-94-1P
                                                                   144891-96-3P
     144891-97-4P
                    144891-98-5P
                                    144891-99-6P
                                                   144892-00-2P
                                                                   144892-01-3P
     144892-02-4P
                    144892-03-5P
                                    144892-04-6P
                                                   144892-05-7P
                                                                   144892-06-8P
     144892-07-9P
                    144892-08-0P
                                    144892-09-1P
                                                   144892-10-4P
                                                                   144892-11-5P
                                                   144892-15-9P
     144892-12-6P
                    144892-13-7P
                                    144892-14-8P
                                                                   144892-16-0P
     144892-17-1P
                    144892-18-2P
                                    144892-19-3P
                                                   144892-20-6P
                                                                   144892-21-7P
     144892-22-8P
                    144892-23-9P
                                    144892-24-0P
                                                   144892-25-1P
                                                                   144892-26-2P
    144892-27-3P
                    144892-28-4P
                                    144892-29-5P
                                                   144892-30-8P
                                                                   144892-31-9P
     144892-32-0P
                    144892-33-1P
                                    144892-34-2P
                                                   144892-35-3P
                                                                   144892-36-4P
                                    144892-39-7P
                                                   144892-40-0P
     144892-37-5P
                    144892-38-6P
                                                                   144892-41-1P
     144892-42-2P
                    144892-43-3P
                                    144892-44-4P
                                                   144892-45-5P
                                                                   144892-46-6P
     144892-47-7P
                                    144892-49-9P
                                                                   144892-51-3P
                    144892-48-8P
                                                   144892-50-2P
                                                                   144892-56-8P
                                    144892-54-6P
                                                   144892-55-7P
     144892-52-4P
                    144892-53-5P
                                    144892-59-1P
                                                                   144892-61-5P
     144892-57-9P
                    144892-58-0P
                                                   144892-60-4P
                                                                   144911-07-9P
     144892-62-6P
                    144892-63-7P
                                    144911-05-7P
                                                   144911-06-8P
     144911-08-0P
                    144911-09-1P
                                    144911-10-4P
                                                   144911-11-5P
                                                                   144911-12-6P
     144911-13-7P
                    144911-14-8P
                                    144911-15-9P
                                                   144911-16-0P
                                                                   144911-17-1P
     144911-18-2P
                    144911-19-3P
                                    144911-20-6P
                                                   144911-21-7P
                                                                   144911-22-8P
    144911-23-9P
                    144911-24-0P
                                    144911-25-1P
                                                   144911-26-2P
                                                                   144911-27-3P
                                    144911-30-8P
                                                   144911-31-9P
     144911-28-4P
                    144911-29-5P
                                                                   144911-32-0P
```

```
144911-34-2P
                                   144911-35-3P
                                                   144911-36-4P
                                                                  144911-37-5P
     144911-33-1P
     144911-38-6P
                    144911-39-7P
                                   144911-40-0P
                                                   144911-41-1P
                                                                  144911-42-2P
                    144911-44-4P
                                   144911-45-5P
                                                   144911-46-6P
                                                                  144911-47-7P
     144911-43-3P
     144911-48-8P
                    144911-49-9P
                                    144911-51-3P
                                                   144911-52-4P
                                                                  144911-53-5P
     144911-54-6P
                    144911-55-7P
                                    144911-56-8P 144911-57-9P
     144911-58-0P 144911-59-1P 144911-60-4P
     144911-61-5P 144911-62-6P 144911-63-7P
     144911-64-8P
                    144911-65-9P
                                   144911-66-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
                                    144911-69-3P
IT
     144911-67-1P
                    144911-68-2P
                                                   144911-70-6P
                                                                  144911-71-7P
                    144911-73-9P
     144911-72-8P
                                   144911-74-0P
                                                   144922-37-2P
                                                                  144922-38-3P
     144922-39-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
ΙT
     1676-63-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with difluoro(pentyl)benzene)
IT
     121219-25-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with ethoxyacetophenone)
TT
     144891-33-8P 144891-34-9P 144891-35-0P
     144891-36-1P 144891-37-2P 144891-38-3P
     144891-39-4P 144911-57-9P 144911-58-0P
     144911-59-1P 144911-60-4P 144911-61-5P
     144911-62-6P 144911-63-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     144891-33-8 CAPLUS
     Benzene, 5-ethoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-
CN
     (9CI) (CA INDEX NAME)
```

$$c = c$$
 $c = c$
 $c = c$
 $c = c$

RN 144891-34-9 CAPLUS
CN Benzene, 1,3-difluoro-5-propoxy-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 $$c = c$$
 $c = c$
 $c = c$
 $c = c$
 $c = c$

RN 144891-36-1 CAPLUS

CN Benzene, 5-ethyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 $c = c$
 $c = c$
 $c = c$

RN 144891-37-2 CAPLUS

CN Benzene, 1,3-difluoro-5-propyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 RN 144891-38-3 CAPLUS

CN Benzene, 5-butyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$c = c$$
 $c = c$
 RN 144891-39-4 CAPLUS

CN Benzene, 1,3-difluoro-5-pentyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$C = C$$

Me- (CH₂) 4

F

O- CF₃

RN 144911-57-9 CAPLUS

CN Benzene, 1,3-difluoro-5-hexyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-(9CI) (CA INDEX NAME)

$$C = C$$

Me- $(CH_2)_5$

F

 $C = C$
 $C = C$
 $C = C$

RN 144911-58-0 CAPLUS

CN Benzene, 1,3-difluoro-5-heptyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

RN 144911-59-1 CAPLUS

CN Benzene, 1,3-difluoro-5-octyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

RN 144911-60-4 CAPLUS

CN Benzene, 1,3-difluoro-5-(pentyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

RN 144911-61-5 CAPLUS

CN Benzene, 1,3-difluoro-5-(hexyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

RN 144911-62-6 CAPLUS

CN Benzene, 1,3-difluoro-5-(heptyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

$$C \equiv C$$

Me- $(CH_2)_6$ -0

F

 $C = C$
 $C = C$
 $C = C$

RN 144911-63-7 CAPLUS

CN Benzene, 1,3-difluoro-5-(octyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl](9CI) (CA INDEX NAME)

$$C = C$$

Me- (CH₂)₇-0

F

O-CF₃

TABLE B-continued

$$C_{n}H_{2n+1} - O - O - C - C - NCS$$

$$PVG-nO-S$$

$$PVG-nO-S$$

$$PVG-NCS$$

$$PVG-nV-S$$

$$PPVU-n-S$$

$$PTG-n(0)-S$$

$$PTG-n(0)-S$$

Concentration/mass-%

8.0

7.0

7.0

6.0

6.0

Use-example 7

[0216] A liquid crystal mixture is realized consisting of:

Use-example 9

[0220] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation

PG-3-AN

PU-3-AN

PU-5-AN

PPVU-2-S

PPVU-3-S

| Compound/Abbreviation | Concentration/mass-% |
|-----------------------|----------------------|
| PTG-5-S | 10.0 |
| PTU-3-S | 15.0 |
| PIU-40-S | 10.0 |
| PVG-5-S | 10.0 |
| PGU-3-S | 10.0 |
| PPU-3-S | 5.0 |
| PPU-4-S | 5.0 |
| PPU-5-S | 5.0 |
| PGIP-3-N | 15.0 |
| PPYP-4N | 15.0 |
| Σ | 100.0 |

[0217] This mixture has the following properties:

| PGP-3-N | 6.0 |
|----------|-------|
| PGIP-3-N | 6.0 |
| PPYP-4N | 8.0 |
| TP-3-S | 4.0 |
| PTG-3-S | 5.0 |
| PVG-5-S | 10.0 |
| PTPG-2-N | 4.0 |
| PPU-CL-S | 4.0 |
| PTP-2O-S | 4.0 |
| PTP-4O-S | 5.0 |
| PTG-20-S | 5.0 |
| PTG-4O-S | 5.0 |
| Σ | 100.0 |

Clearing point (T(N,I))/° C: 126.5

Smectic to nematic <-10

transition point (T(S,N))/° C:
n_e (20° C., 589.3 nm): 1.9475

Δn (20° C., 589.3 nm): 0.4016

Use-example 8

[0221] This mixture has the following properties:

| Clearing point (T(N,I))/° C.: | 135.0 | |
|------------------------------------|--------|--|
| n _e (20° C., 589.3 nm): | 1.9906 | |
| Δn (20° C., 589.3 nm): | 0.4511 | |
| | | |

[0218] A liquid crystal mixture is realized consisting of:

Comparative Use-example 1

[0222] A liquid crystal mixture is realized consisting of:

| Compound/Abbreviation | Concentration/mass-% |
|-----------------------|----------------------|
| PIG-5-S | 10.0 |
| PIU-3-S | 13.0 |
| PTU-40-S | 10.0 |
| PVG-5-S | 11.0 |
| PGU-3-S | 10.0 |
| PPU-3-S | 5.0 |
| PPU-4-S | 5.0 |
| PPU-5-S | 5.0 |
| PGIP-3-N | 12.0 |
| PPYP-4N | 13.0 |
| PVG-V-S | 6.0 |
| ι Σ | 100.0 |

[0219] This mixture has the following properties:

| Compound/Abbreviation | Concentration/mass-% |
|-----------------------|----------------------|
| K6 | 12.0 |
| К9 | 4.0 |
| K15 | 29.6 |
| M9 | 8.8 |
| T15 | 8.0 |
| PGIP-3-N | 20.0 |
| BB2I | 5.6 |
| BCH-5 | 12.0 |
| | 100.0 |

[0223] This mixture has the following properties:

| Clearing point (T(N,I))/° C.: | 125.0 |
|--|--------|
| Smeetic to nematic transition point (T(S,N))/° C.: | <-10 |
| n _e (20° C., 589.3 nm): | 1.9623 |
| Δn (20° C., 589.3 nm): | 0.4153 |

| Clearing point (T(N,I))/° C: | 113.0 |
|------------------------------|--------|
| n, (20° C. 589.3 nm): | 1.8160 |
| Δn (20° C. 589.3 nm): | 0.2860 |
| € (20° C., 1 kHz): | 22.8 |
| Δε (20° C., 1 kHz): | 17.3 |

Comparative Use-example 2

[0224] A liquid crystal mixture is realized consisting of:

| Compound/Abbreviation | Concentration/mass-% |
|-----------------------|----------------------|
| ME2N.F | 10.00 |
| PPTUI-2-4 | 8.45 |
| PPTUI-3-2 | 5.16 |
| PPTUI-3-4 | 15.82 |
| PPTUI-4-4 | 35.54 |
| PPTUI-5-2 | 7.25 |
| PPTUI-5-4 | 17.78 |
| E | 100.00 |

[0225] This mixture has the following properties:

| | | _ |
|-------------------------------|---------|---|
| Clearing point (T(N,I))/° C.: | 145° C. | |
| Δn (20° C., 589.3 nm): | 0.336 | |
| طا (20° C., 1 kHz): | 9.8 | |
| Δε (20° C., 1 kHz): | 6.5 | |

Comparative Use-example 3

[0226] A liquid crystal mixture is realized consisting of:

| Compound/Abbreviation | Concentration/mass-% |
|-----------------------|----------------------|
| GGP-5-GL | 16.0 |
| PGIGI-3-CL | 6.0 |
| BCH-2F.F | 14.0 |
| BCH-3F.F | 15.0 |
| BCH-5F.F | 14.0 |
| BCH-3F.F.F | 14.0 |
| CGU-2-F | 6.0 |
| CGU-3-F | 6.0 |
| CGU-5-F | 6.0 |
| CBC-33F | 3.0 |
| E | 100.0 |

[0227] This mixture has the following properties:

| Clearing point (T(N,I))/° C.: | 81.0 |
|------------------------------------|--------|
| Smectic to nematic | <-30 |
| transition point (T(S, N))/° C: | |
| n _e (20° C., 589.3 nm): | 1.6711 |
| Δn (20° C. 589.3 nm): | 0.1603 |
| d (20° C., 1 kHz): | 14.6 |
| Δε (20° C. 1 kHz): | 9.9 |

What is claimed is:

- 1. A liquid crystal medium, comprising:
- a strongly dielectrically positive liquid crystal component A, containing one or more liquid crystal compounds with a terminal isothiocyanate group and having a Δn of more than 0.30 at 20° C. and 589.3 nm, and
- a dielectrically positive component B containing of one or more terminally polar substituted bi- or terphenyl compounds.

2. A liquid crystal medium according to claim 1, wherein the dielectrically positive liquid crystal component A comprises one or more compounds of formula I

$$R^{1}$$
 Z^{11} Z^{12} Z^{12} Z^{12} Z^{13} Z^{13} Z^{14} Z^{15}

wherein

R¹ is n-alkyl, or n-alkoxy with 1 to 10 C-atoms, alkenyl, alkenyloxy or alkoxyalkyl with 2 to 7 C-atoms or CN, NCS, halogen, or alkyl, alkenyl, alkoxy, alkenyloxy or alkoxyalkyl substituted by one or more halogens,

Each, independently of each other, are

Z¹¹ and Z¹² each are independent of each other a single bond or trans —CH=CH—, provided that when n¹ is 0, Z¹² is a single bond

n1 is 0 or 1.